

Ground-state phase diagram of the Kondo lattice model on triangular-to-kagome lattices

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Abstract

We investigate the ground-state phase diagram of the Kondo lattice model with classical localized spins on triangular-to-kagome lattices by using a variational calculation. We identify the parameter regions where a four-sublattice noncoplanar order is stable with a finite spin scalar chirality while changing the lattice structure from triangular to kagome continuously. Although the noncoplanar spin states appear in a wide range of parameters, the spin configurations on the kagome network become coplanar as approaching the kagome lattice; eventually, the scalar chirality vanishes for the kagome lattice model.

PACS numbers: 71.10.Fd, 71.27.+a, 75.10.Lp

Keywords: spin scalar chirality, triangular lattice, kagome lattice, double exchange model

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I. INTRODUCTION

Recently, unusual magnetic orderings have been of intensive research interest in geometrically-frustrated spin-charge coupled systems. In particular, a spin scalar chiral ordering has attracted considerable attention. A typical example was theoretically discussed for the Kondo lattice model on a kagome lattice [1]. It was shown that a noncoplanar spin ordering with the $\mathbf{q} = \mathbf{0}$ three-sublattice structure induces an unconventional anomalous Hall effect through the Berry phase mechanism. Another example has been recently attracting attention — a scalar chiral ordering with a four-sublattice noncoplanar spin configuration on a triangular lattice [2–6]. The particular order appears in two regions, near $3/4$ filling and $1/4$ filling [3]. While the former was deduced from the perfect nesting of the Fermi surface [2], the latter is unexpected from the nesting scenario; instead, it was clarified that the $1/4$ -filling chiral state is induced by a critical enhancement of effective positive biquadratic interactions through the generalized Kohn anomaly [6].

The four-sublattice noncoplanar order on the triangular lattice can be viewed as an extension of the three-sublattice one on the kagome lattice. The kagome lattice is obtained by depleting $1/4$ sites periodically in the triangular lattice. When omitting $1/4$ sites periodically from the four-sublattice order on the triangular lattice, one ends up with the $\mathbf{q} = \mathbf{0}$ three-sublattice order with a particular solid angle of three spins on the kagome lattice. The stability of the four-sublattice order was studied in detail on the triangular lattice [3], but that of the three-sublattice order was not investigated on the kagome lattice; the spin pattern was set by hand as an internal field for itinerant electrons [1].

In this contribution, we investigate the stability of noncoplanar spin ordering in the Kondo lattice model on the kagome lattice from the viewpoint of connection to the four-sublattice order on the triangular lattice. We consider a continuous change of the lattice structure from triangular to kagome by modulating the electron hopping between the $1/4$ sites and the neighboring sites. By using a variational calculation for the ground state similar to the previous studies [3, 7], we clarify the parameter regions where the noncoplanar chiral state becomes stable.

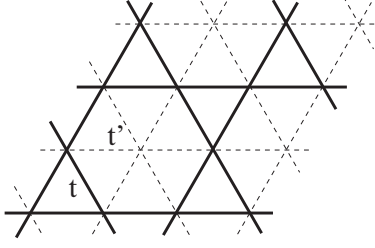


FIG. 1: Schematic picture of the triangular-to-kagome lattice. The transfer integrals are periodically modulated by changing the ratio t'/t so that the network connected by t forms the kagome lattice at $t' = 0$.

II. MODEL AND METHOD

We consider the Kondo lattice model on a triangular lattice with a modulation of electron hopping to connect the triangular and kagome lattice structures, as shown in Fig. 1. We call this the triangular-to-kagome lattice hereafter. The Hamiltonian is given by

$$\mathcal{H} = - \sum_{\langle i,j \rangle, \alpha} t_{ij} (c_{i,\alpha}^\dagger c_{j,\alpha} + \text{h.c.}) - J_H \sum_{i,\alpha,\beta} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta} \cdot \mathbf{S}_i, \quad (1)$$

where $c_{i,\alpha}^\dagger$ ($c_{i,\alpha}$) is a creation (annihilation) operator of conduction electron at site i with spin α , $\boldsymbol{\sigma}$ is the Pauli matrix, and \mathbf{S}_i is a localized moment at site i . The hopping matrix t_{ij} takes $t(=1)$ or t' ($0 \leq t' \leq 1$) as being the triangular-to-kagome lattice; $t' = t$ ($t' = 0$) corresponds to the triangular (kagome) lattice. The sum in the first term is taken for the nearest-neighbor sites on the triangular-to-kagome lattice. The sign of the spin-charge coupling J_H does not matter, since we treat \mathbf{S}_i as a classical spin.

Following the previous studies by the authors [3, 7], we investigate the ground state of the model given by eq. (1) by a variational calculation while varying the electron density $n = \frac{1}{N} \sum_{i\alpha} \langle c_{i,\alpha}^\dagger c_{i,\alpha} \rangle$ (N is the total number of sites), J_H , and t' . We compare the grand-canonical potentials $\Omega = \langle \mathcal{H} \rangle - \mu n$ at $T = 0$ (μ is the chemical potential) for different ordered states of the localized spins, and determine the most stable ordering. In the calculation, we consider 13 different types of ordered states, up to a four-site unit cell, as shown in Fig. 2. For the states (2b), (3b), (3c), (3d), and (4d), we optimize the canting angle θ .

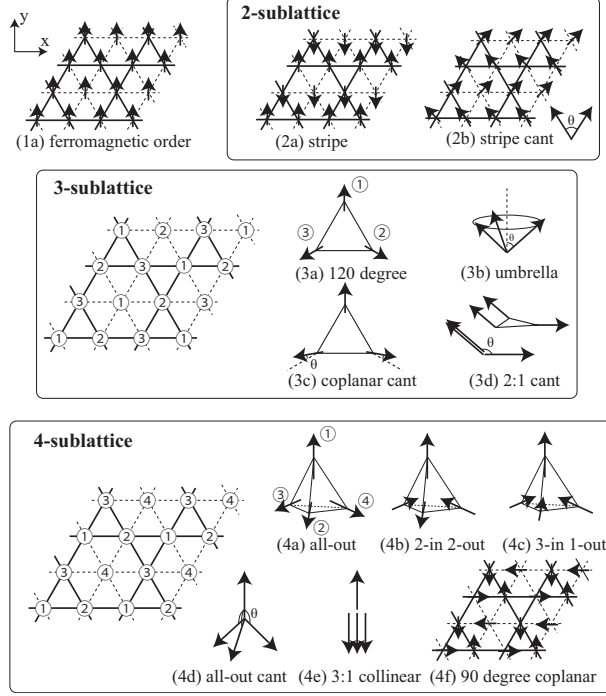


FIG. 2: Ordering patterns on the triangular-to-kagome lattice: (1a) a ferromagnetic, (2a) a two-sublattice collinear stripe, (2b) a stripe order with a canting angle θ , (3a) a three-sublattice 120° noncollinear, (3b) a noncoplanar umbrella-type order with angle θ (canted in the normal direction to the coplanar plane from the 120° order), (3c) a coplanar order with a canting angle θ for two spins from 120° order, and (3d) a 2:1-type order with two parallel spins that have an angle θ to the remaining one. (4a) a four-sublattice all-out-type, (4b) a two-in two-out-type, (4c) a three-in one-out-type order, (4d) an all-out-type order with a canting angle θ for three spins, (4e) a 3:1 collinear order, and (4f) four-sublattice coplanar 90° spiral order. Note that (2b) with $\theta = \pi$, (3b) with $\theta = \frac{\pi}{2}$, (3c) with $\theta = 0$, (4d) with $\theta = \cos^{-1}(-1/3)$, $\theta = \cos^{-1}(+1/3)$, and $\theta = \pi$ are equivalent to (2a), (3a), (3a), (4a), (4c), and (4e), respectively.

III. RESULTS AND DISCUSSION

Figure 3 shows the results of the phase diagram as functions of n and J_H at (a) $t' = 0.9$, (b) 0.8, (c) 0.6, (d) 0.4, (e) 0.2, and (f) 0.1. Here, we focus on the changes of the four-sublattice chiral phases (4a) and (4d), which are candidates of the chiral phase with the $\mathbf{q} = \mathbf{0}$ three-sublattice order in the kagome limit $t' = 0$. In the isotropic triangular lattice case ($t' = t = 1$), the state (4a) appears dominantly near $1/4$ - and $3/4$ -filling, while the canted state (4d) is not stable [3]. The $1/4$ -filling one is stabilized in a wider range of

parameters than the 3/4-filling one.

First, we focus on the change of the state (4a) near 1/4-filling. As we introduce a small modulation to the triangular lattice by decreasing t' from $t' = 1$, the (4a) region becomes narrower, and instead, the state (4d) is induced around (4a). When t' is further decreased, the state (4a) is taken over by (4d) around $t' \simeq 0.5$; (4d) region, however, is also narrowed. Eventually, the chiral states vanish in the limit of the kagome lattice ($t' = 0$). We note that the insulating state at $n = 1/4$ remains robust down to $t' \simeq 0.3$, in sharp contrast to the 3/4-filling one described below, reflecting the difference of the origins of 1/4- and 3/4-filling states [6].

Next, we consider the change near 3/4 filling. When we reduce t' from $t' = 1$, the chiral state (4a) at 3/4 filling is quickly destabilized, in sharp contrast to the 1/4-filling case. This is because the state (4a) is stabilized by the perfect nesting of the Fermi surface present at $t = t'$ [2], which disappears for $t' < t$. Instead, the state (4d) appears in the region of $n < 3/4$. As decreasing t' , (4d) is intervened by the state (3a) appearing for $t' \lesssim 0.4$. It is noteworthy that the state (4d) spreads as t' decreases, and is stabilized in a wide range of parameters near 1/2 filling for $t' \lesssim 0.2$. Although this noncoplanar phase shows a finite scalar chirality and the associated anomalous Hall effect, the scalar chirality defined on the kagome network approaches zero as $t' \rightarrow 0$ because the canting angle θ approaches $\pi/2$. In the limit of the kagome lattice $t' = 0$, the spins on the kagome network become coplanar with forming the $\mathbf{q} = \mathbf{0}$ 120° order, and hence, the scalar chirality vanishes.

Consequently, our results indicate that the chiral phase considered by Ohgushi *et al.* [1] is not realized on a kagome lattice within the present model, although a related chiral phase is induced by introducing the connection to the triangular lattice by a nonzero t' . The present results, however, do not deny the possibility of another form of a chiral state or noncoplanar ordering on the kagome lattice, since the present calculation is limited by the unit cell sizes considered in the variational states in Fig. 2. For example, it was recently pointed out that a noncoplanar order with a larger unit cell can be stabilized by the perfect nesting at 1/3 filling [9]. To extend our analysis by taking account of larger unit cells is left for future study.

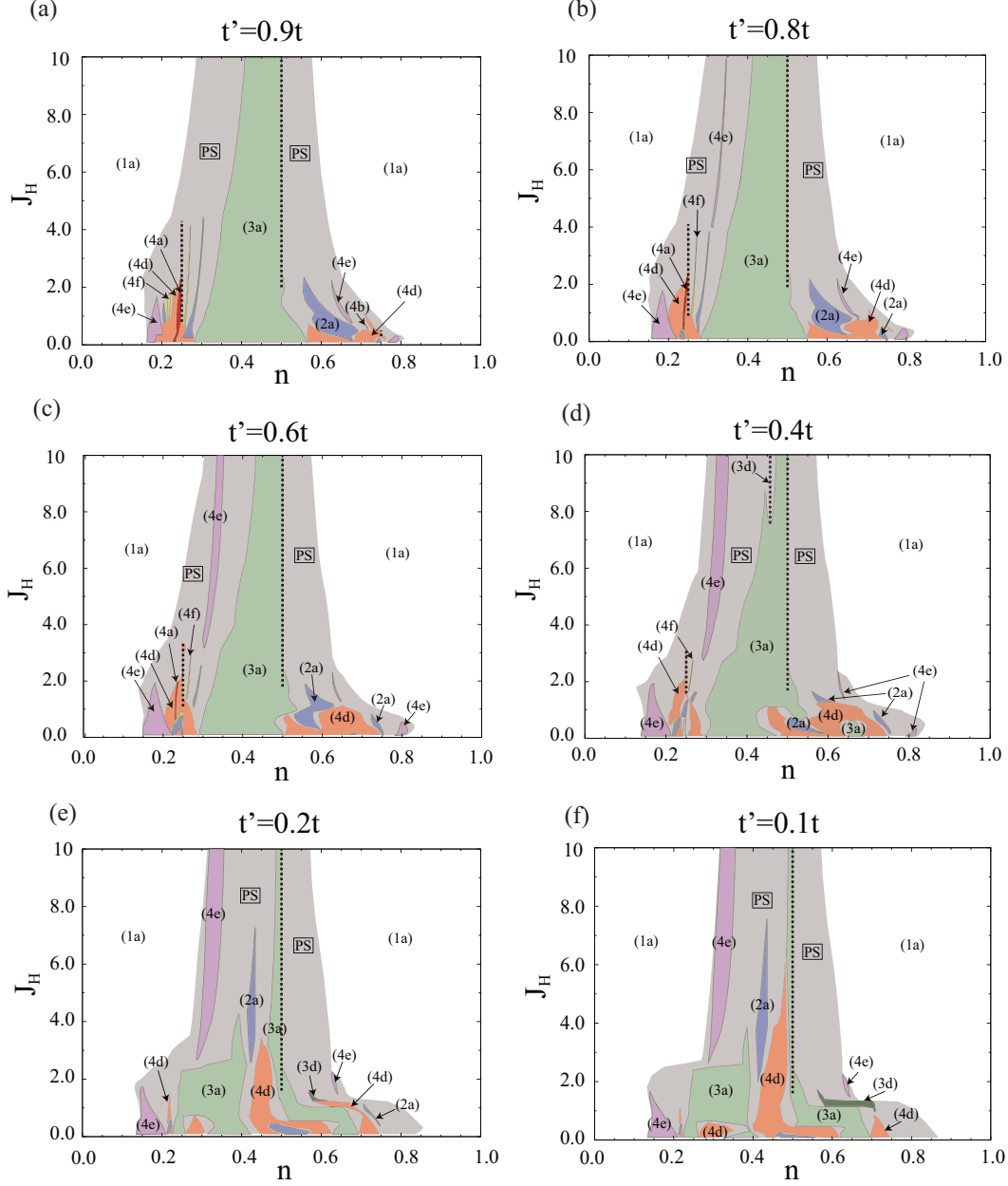


FIG. 3: (Color online) Ground-state phase diagrams on the triangular-to-kagome lattices at (a) $t' = 0.9$, (b) 0.8 , (c) 0.6 , (d) 0.4 , (e) 0.2 , and (f) 0.1 . The vertical dashed lines at $n = 1/4$, $1/2$, and $3/4$ show gapful insulating regions [8]. PS indicates a phase-separated region.

IV. CONCLUSION

We have investigated the ground-state phase diagram of the Kondo lattice model with classical localized moments on triangular-to-kagome lattices. Using the variational calculations upon a variety of ordered states up to a four-site unit cell, we identified the parameter

regions where the spin scalar chiral states with noncoplanar spin configuration are stabilized. The chiral phases, originating in those near $1/4$ and $3/4$ fillings in the isotropic triangular lattice case, remain in a wide range of parameters as the lattice structure is modulated continuously to the kagome lattice. In the limit of kagome lattice, $t' = 0$, however, the spin configurations become coplanar on the kagome network and the scalar chirality vanishes in the entire region of the phase diagram.

Acknowledgments

We acknowledge helpful discussions with Takahiro Misawa, Masafumi Udagawa, and Youhei Yamaji. Y.A. gratefully thanks Satoru Hayami for his fruitful comments. Y.A. is supported by Grant-in-Aid for JSPS Fellows. This work was supported by Grants-in-Aid for Scientific Research (Grants No. 19052008, No. 21340090, and No. 24340076), Global COE Program “the Physical Sciences Frontier”, the Strategic Programs for Innovative Research (SPIRE), MEXT, and the Computational Materials Science Initiative (CMSI), Japan. The computation in this work has been done using the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

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